Electronic Supplementary Material (ESI) for Dalton Transactions.

Electron Deficient Nonplanar β-Octachlorovanadylporphyrin as Highly Efficient and Selective Epoxidation Catalyst for Olefins

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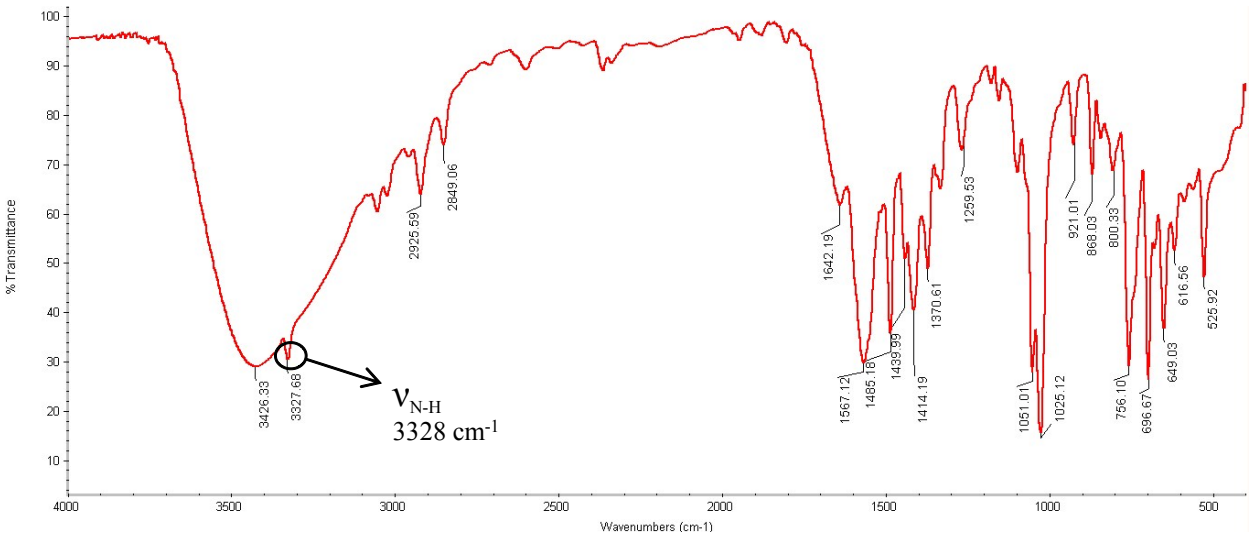
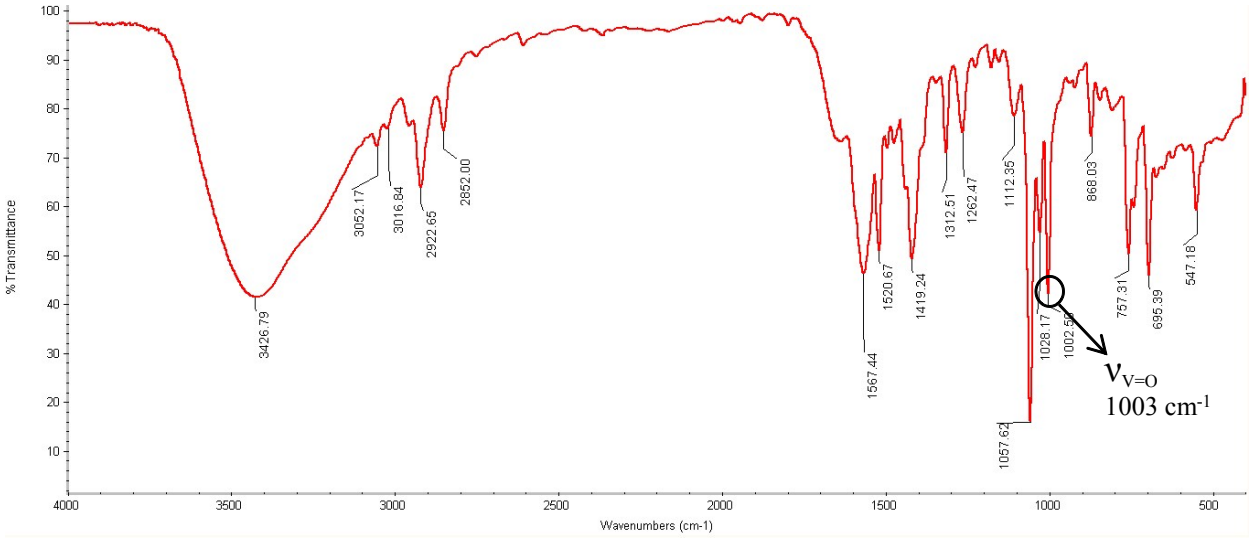
Table of Contents

	Page No
Figure S1. FT-IR spectra of (a) H_2TPPCl_8 and (b) $VOTPPCl_8$ using KBr pellets.	2
Figure S2. MALDI-TOF mass spectra of $VOTPPCl_8$ using HABA matrix. Insets show the molecular ion peaks obtained from experiment and simulation.	3
Table S1. Selected bond lengths (A) and bond angles (°) for the B3LYP/6-311G(d,p) optimised geometry of **$VOTPPCl_8$ in CH_3CN**. The values if the given figure represent the deviation of atoms from the porphyrin mean plane formed by 24 atoms core.	4
Figure S3. B3LYP/LANDLD2Z optimized geometry showing (a) top and (b) side view of **H_2TPPCl_8 in CH_3CN**. In side view, β-chloro and *meso*-phenyl groups are not shown for clarity.	5
Table S2. Selected bond lengths (Å) and bond angles (°) for the B3LYP/6-311G(d,p) optimised geometry of H_2TPPCl_8 in CH_3CN. The values if the given figure represent the deviation of atoms from the porphyrin mean plane formed by 24 atoms core.	5
Figure S4. DPV of $VOTPPCl_8$ in CH_2Cl_2 indicating one electron redox processes.	6
Figure S5. CV and DPV of $VOTPPCl_8$ in CH_2Cl_2 containing 0.1 M $TBAPF_6$ at 298 K.	7
Figure S6. Thermogram (TG), Differential thermal analysis (DTA) and Differential thermogram (DTG) of $VOTPPCl_8$ at the heating rate of 10 °C /minute scanned from 25 °C to 1000 °C.	8
Figure S7. MALDI-TOF mass spectra of $VOTPPCl_8$ in presence of hydrogen peroxide and sodium bicarbonate using HABA matrix.	9
Figure S8. MALDI-TOF mass spectra of the reaction mixture after addition of the cyclohexene to oxido- peroxidovanadium(V) intermediate using HABA matrix.	9
Figure S9. UV-Visible spectra of $VOTPPCl_8$ in CH_2Cl_2 (before catalysis) and in CH_3CN (after catalytic reaction) at 298 K.	10

(a)



(b)



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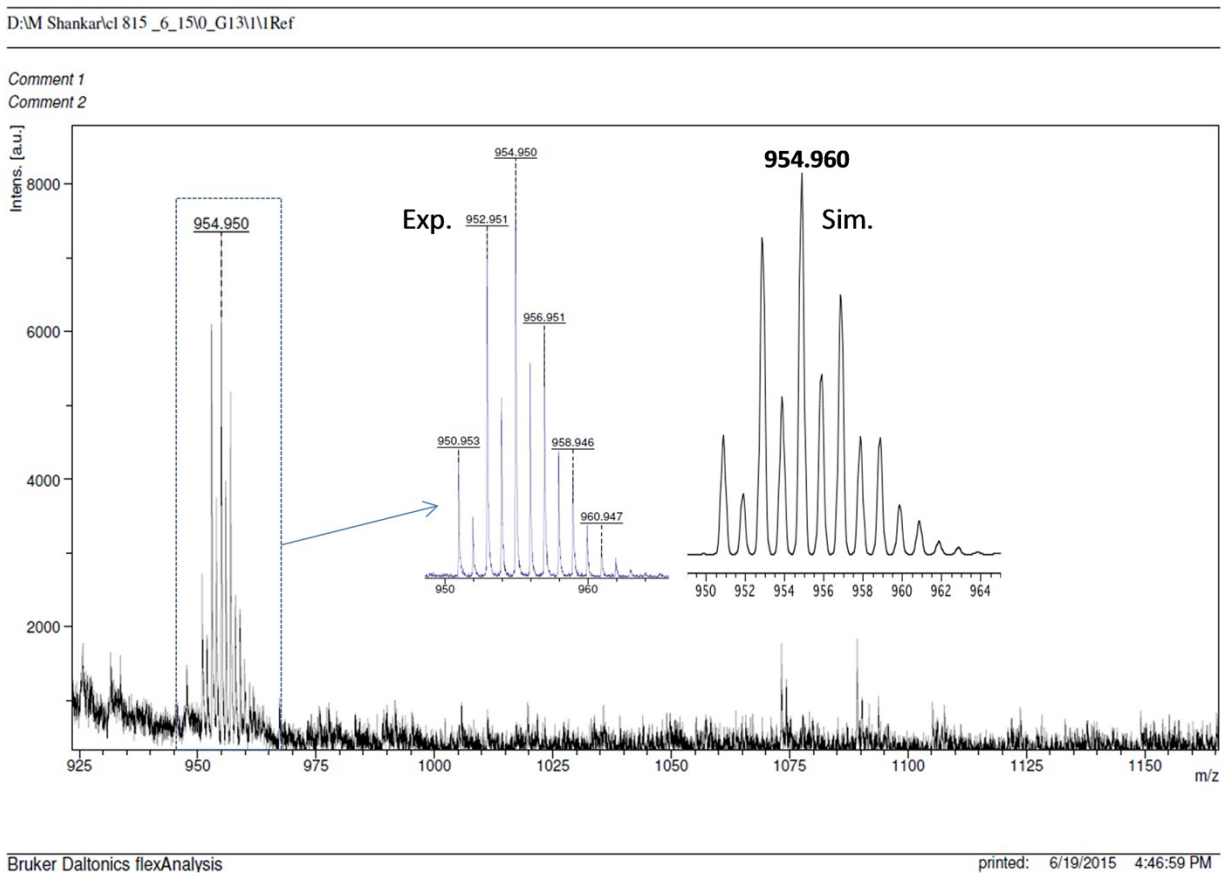

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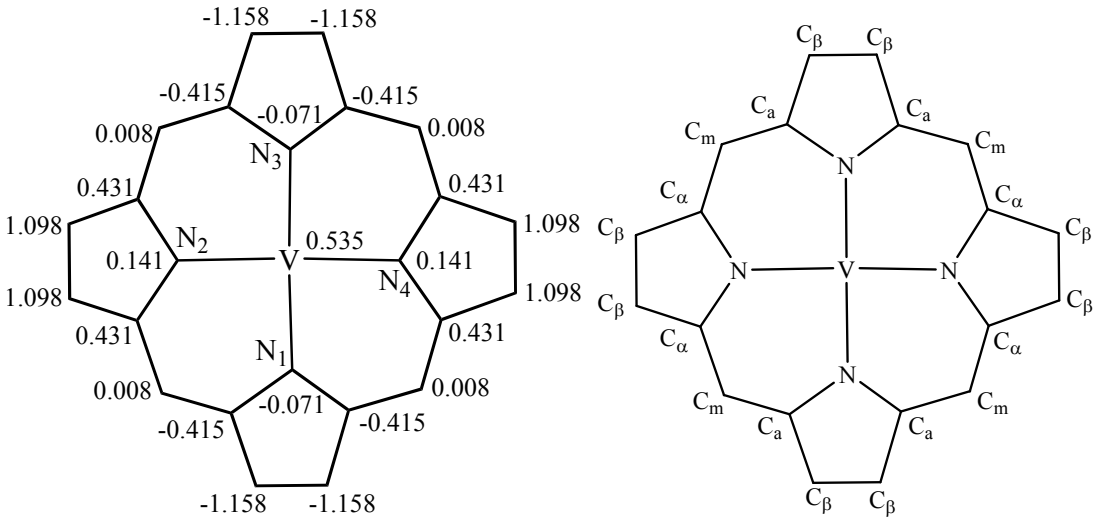
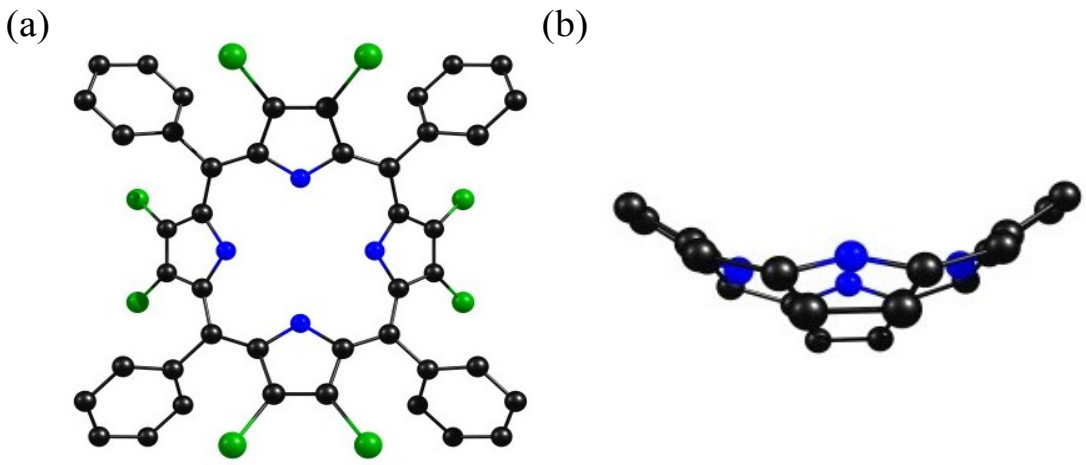


Bond Length (Å)		Bond Angle (°)	
V-N	**2.065**	**M-N-C_α**	**123.00**
V-O	1.602	N-M-N	153.06
N-C_α	1.402	**N-C_α-C_m**	**123.80**
C_α-C_β	1.452	N-C_α-C_β	107.82
C_β-C_β	**1.375**	**C_β- C_α-C_m**	**128.16**
C_α-C_m	1.413	C_α-C_β-C_β	107.89
ΔC_β (Å)[a]	**1.128**	C_α-N-C_α	107.90
Δ24 (Å)[b]	**0.535**		
ΔMetal (Å)[c]	**0.515**		

[a]Deviation of β-pyrrole carbons from porphyrin mean plane formed by 24-atom core

[b]Deviation of 24 atoms from the porphyrin mean plane

[c]deviation of metal atom (V^{IV}) from the porphyrin mean plane



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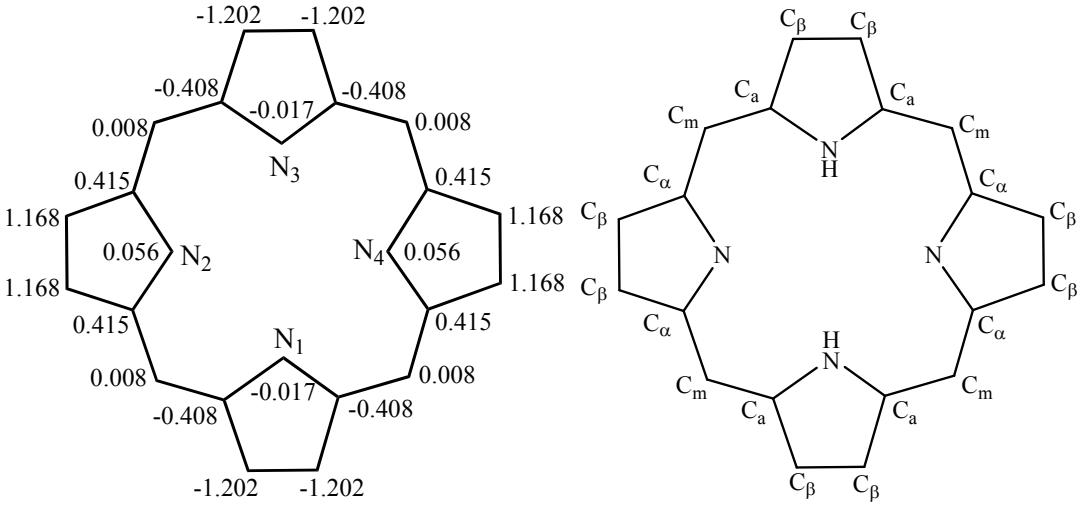
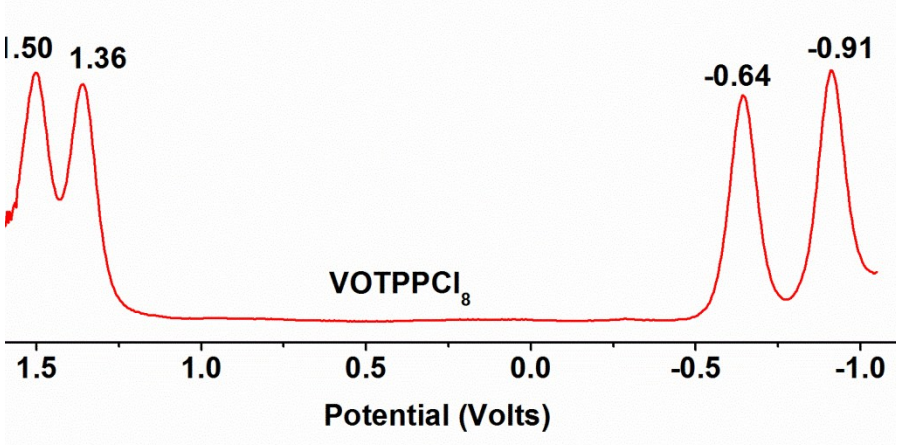


Bond Length (Å)		Bond Angle (°)	
N-C_α	1.389	**N-C_α-C_m**	**124.10**
C_α-C_β	1.457	N-C_α-C_β	106.74
C_β-C_β	**1.377**	**C_β- C_α-C_m**	**129.03**
C_α-C_m	1.422	C_α-C_β-C_β	108.02
ΔC_β (Å)[a]	**1.185**	C_α-N-C_α	110.15
Δ24 (Å)[b]	**0.674**		

[a]Deviation of β-pyrrole carbons from porphyrin mean plane formed by 24-atom core.

[b]Deviation of 24 atoms from the porphyrin mean plane.



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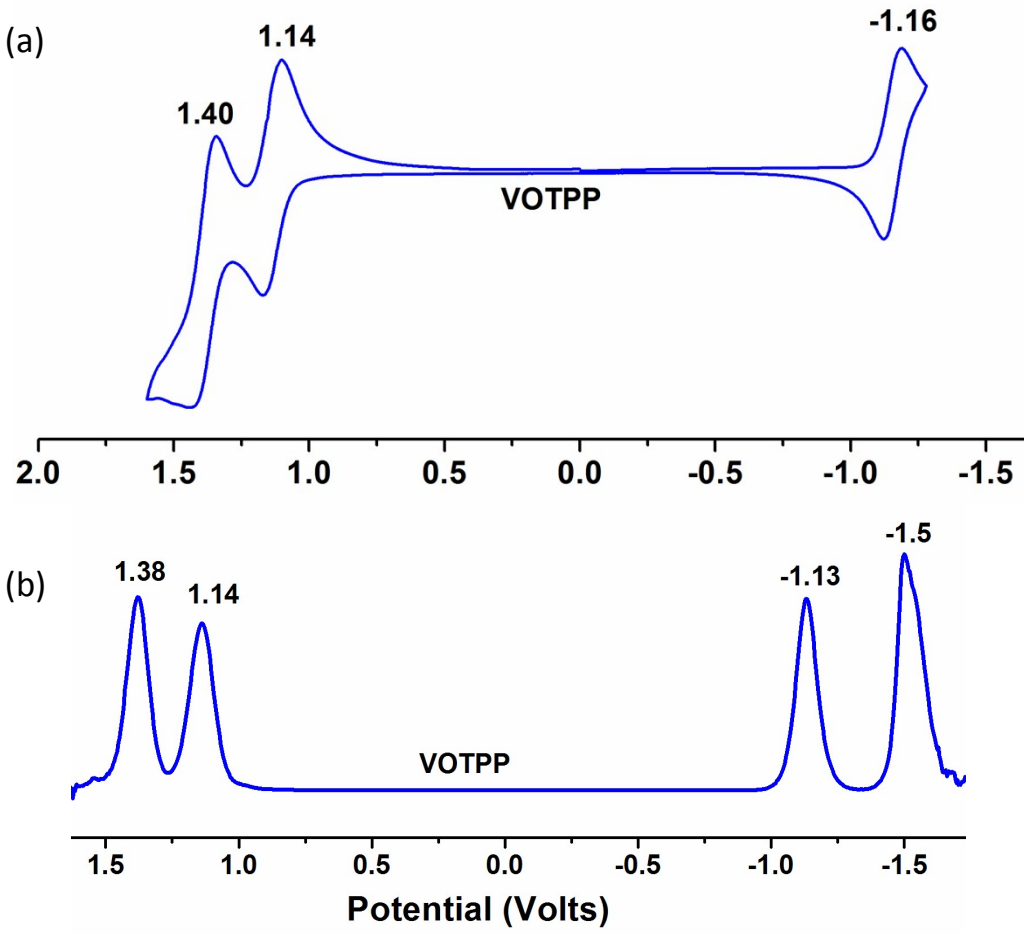
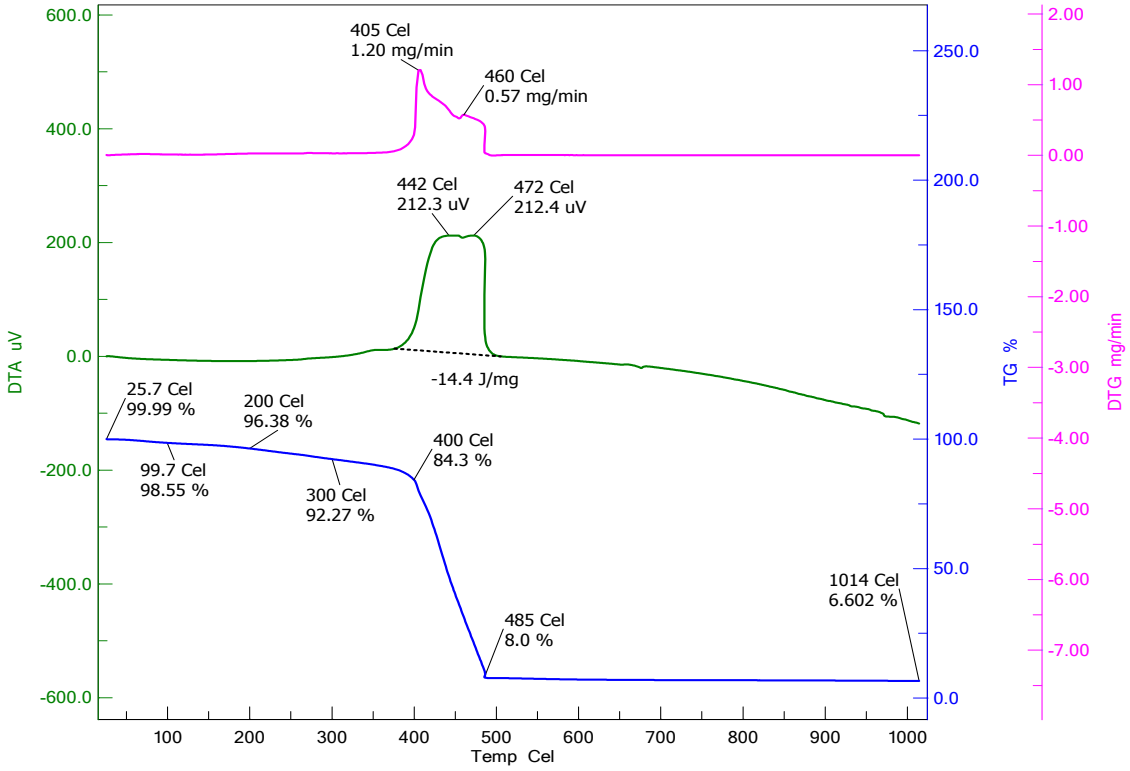


Figure S5. CV and DPV of $VOTPPCl_8$ in CH_2Cl_2 containing 0.1 M $TBAPF_6$ at 298 K.



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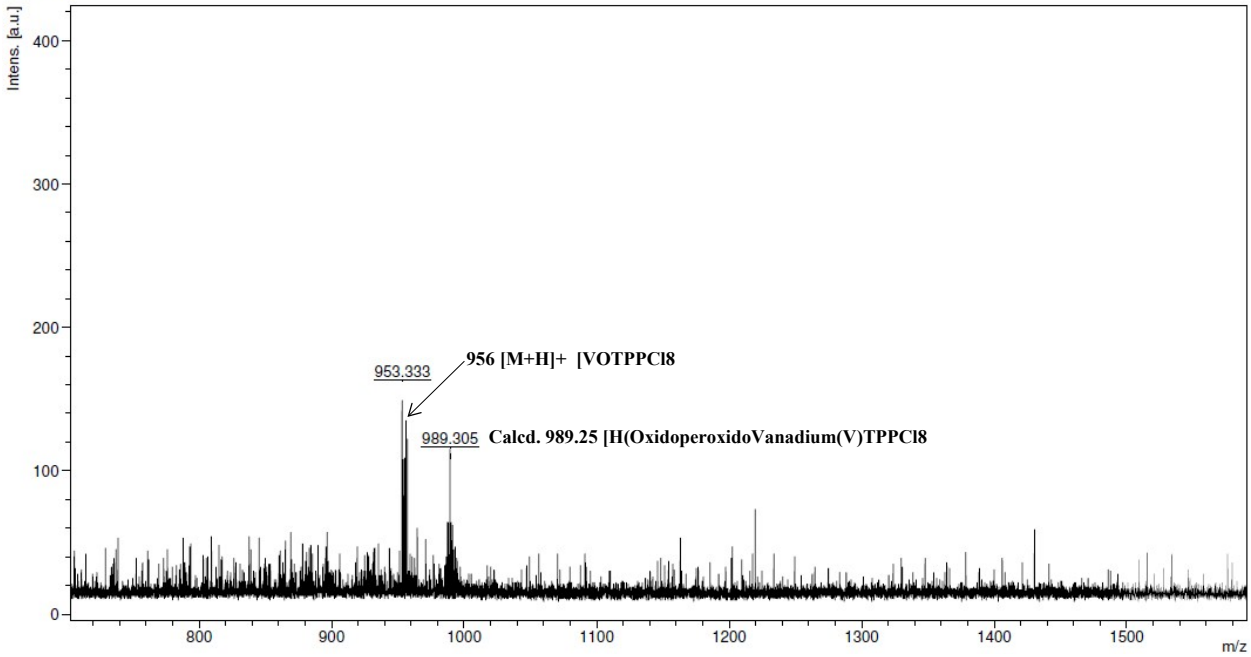


Figure S7. MALDI-TOF mass spectra of $VOTPPCl_8$ in presence of hydrogen peroxide and sodium bicarbonate using HABA matrix.

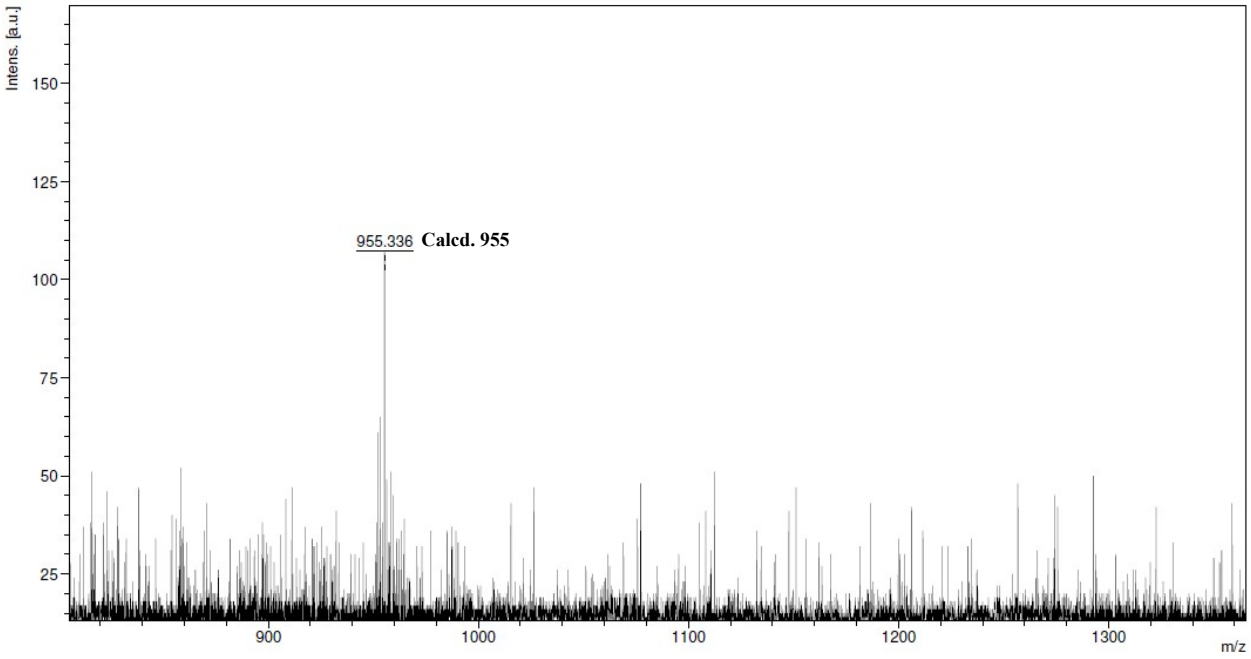
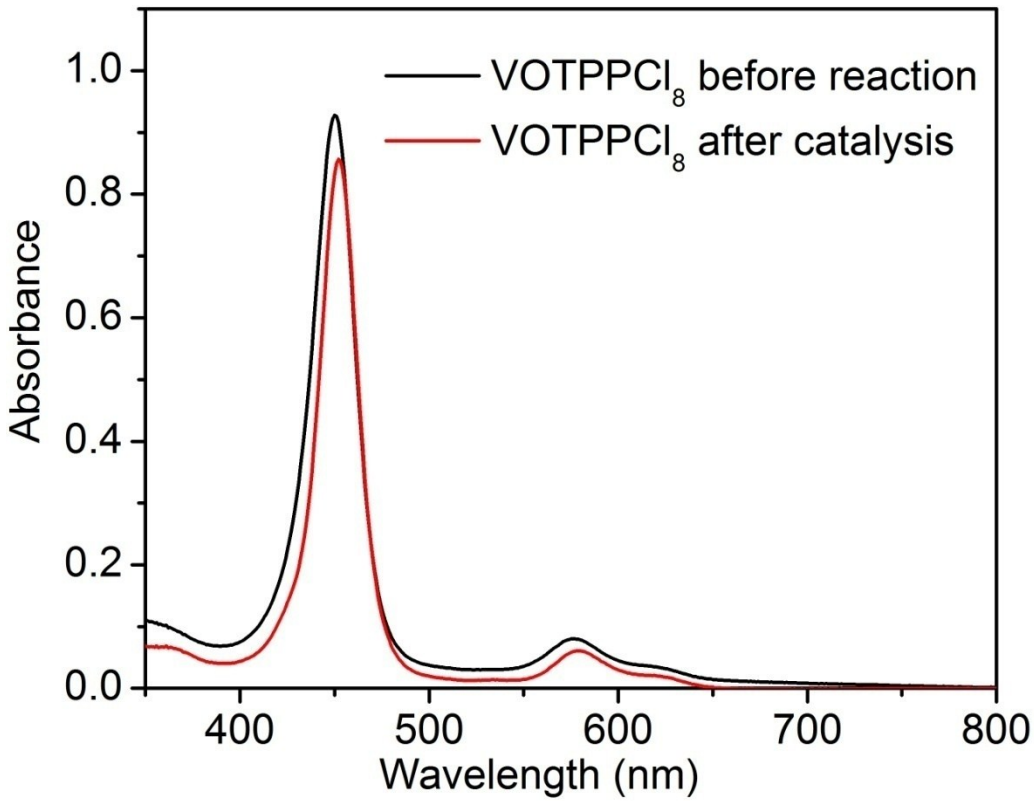


Figure S8. MALDI-TOF mass spectra of the reaction mixture after addition of the cyclohexene to oxido-peroxidovanadium(V) intermediate using HABA matrix.



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